

Status Report #5

for

NASA Research Grant NsG-287 to Haverford College

Title: Wave Functions and Transition Probabilities for Light
Atoms and Highly Ionized Ions.

Interval Covered by this Report: August 1, 1965 - January 31, 1966.

Institution Sponsoring the Work: Haverford College, Haverford, Penna.

Department: Astronomy

Principal Investigator: Dr. Louis C. Green

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Present State of the Work:

1. Wave functions and energies for He I

a) Approximately one hundred requests have been received for reprints of the paper mentioned in the previous status report, "Wave Functions for the Excited States of Neutral Helium", which appeared in the July 19 issue of the Physical Review.

b) The preparation of the paper on "Non-Autoionizing Doubly Excited States of H^- and He I" which was mentioned in the previous status report has been stopped temporarily while a search is made for the cause of a disagreement between the earlier results obtained on an IBM 7094 and those found with a modification of the same program on a CDC 6600.

2. Transition probabilities in He I

a) Both galley proof and page proof have been received and corrected for the article, "Oscillator Strengths and High Accuracy Wave Functions for Neutral Helium", which is to appear in the transactions of Symposium 26 of the International Astronomical Union.

b) The paper, "Oscillator Strengths for Singlet and Triplet Series in Neutral Helium", has been accepted for publication in the April issue of the Astrophysical Journal.

c) A program has been written, tested, and applied which attempts to derive improved transition probabilities by minimizing the difference between the values obtained from the dipole length, velocity, and acceleration expressions. Analytic wave functions which have been chosen by the minimum principle, with the variation of both linear and non-linear parameters, to give excellent values of the energy are introduced into the three expressions. The linear parameters are then varied to minimize the difference in the oscillator strength as computed in any two, or in all three, ways. As would be expected, variations in the parameters affect the transition probabilities more than the energies, since the latter are minima. The success of this procedure has not as yet been as great as was hoped but several ideas are available which may lead to better results.

3. Ground state wave function for Ca I

For several years Dr. Chen and the Principal Investigator have been trying to work out an effective procedure for obtaining wave functions which include exchange throughout and correlation between the valence electrons. A large amount of time has been devoted to a method which starts out from numerical Hartree self-consistent field wave functions with exchange. Analytic correlation terms of rather general

type are then added and a multi-dimensional Schmidt process is applied to restore the orthogonality with the wave functions of the core electrons. This procedure leads to very laborious calculations which have not as yet resulted in the desired improvement in the energies obtained. Nevertheless the objective of obtaining wave functions with exchange between all electrons and correlation between those outside closed shells seems very desirable. A new approach to the problem has therefore been undertaken. Non-diagonal Lagrangian multipliers are employed to maintain the strong orthogonality conditions. Up to the date of this report, self-consistency has not been pushed beyond the second iteration. However, if present indications are fulfilled, improvements in the energy beyond those originally hoped for will shortly be obtained.

4. Ground state wave function for He I

The attempt to represent the He I ground state wave function with linear combinations of antisymmetrized central field functions has led to a reduction in the error in the energy by 85% over the best previous published value obtained from a configuration interaction calculation. It has been decided to stop the calculations at this point and to prepare a paper on the results within the next month for submission to the Physical Review. There is a very large amount of information available in the various calculations which have been performed in connection with this problem. The interest of this undertaking was primarily methodological, and the results obtained will allow tests to be applied to some of the suppositions which have been expressed from time to time in the literature in regard to the rate of convergence which can be obtained with central field functions.

5. Wave functions, energies, and f-values for Li II and heavier ions

The generation of high accuracy wave functions for Li II has been the sustaining problem in recent months while other calculations were being pressed. It now seems that this work should be carried through to completion in a reasonable time interval and that work on heavier ions of interest should be begun.

6. Analysis of the Fe II spectrum

a) Plates: Just after the close of the period under review, Prof. A. G. Shenstone of Princeton took a series of Schuler tube exposures of Fe II covering the wavelength range from about 2100 to 6600 angstroms. These plates appear to be excellent. The lines are sharp, as one expects from the hollow cathode discharge, and the exposure times are such as to give measurable lines in all but the strongest cases. These plates are clearly an outstanding addition to the material on which to base the analysis.

b) Wavelength reductions: In the far ultraviolet region, wavelength standards are still relatively few. Furthermore

many of the so-called standards have had their wavelengths determined from plates taken at far lower dispersion than that which characterizes the plates taken for the Principal Investigator at the National Bureau of Standards. The problem of obtaining the maximum of information from those plates which were taken in the far ultraviolet thus becomes difficult. Several procedures have been tried in the hope of finding the most effective methods of plate reduction, but a clear decision between various procedures has not yet been obtained. Unfortunately the emulsion employed on many of the NBS plates is such as to scatter the incident ultraviolet rather strongly. As a result many of the stronger lines are not accurately measurable on any of the plates presently available. An added difficulty in what might be thought to be an essential routine part of the work has arisen from the plate measuring engine. The Grant instrument is in many ways a superb instrument, but there has been some slight trouble with drift and the associated electronics and automatic features have not worked as well as was hoped. With further effort, these difficulties will probably be overcome.

c) Analysis: Machine programs have been written to make preliminary surveys of the wavelength lists in search of constant differences. These programs seem to work very well, but their usefulness in the far ultraviolet has been reduced by the difficulties encountered in obtaining sufficiently high accuracy in the wave numbers. In the violet, ultraviolet, and far ultraviolet, the plates are very rich, so that change coincidences of wave number differences are numerous. A substantial part of the richness originates in the simultaneous presence on the plates of many lines of Fe I and Fe III in addition to those of Fe II. However the variety of excitation conditions employed in the various exposures available should allow for the removal from the line lists of many of these intruders.

7. Spectrum of the peculiar A star HD 188041

Machine programs have been written and applied to the problem of line identification. Initially a large section of Charlotte Moore's Multiplet Table of Astrophysical Interest has been punched on cards. The procedure is then to feed selected multiplets together with a wavelength list from the stellar spectrum into the computer. The output of this ~~first run is the most probable value of the radial velocity to be used with this set of multiplets.~~ If the radial velocity to be used with other multiplets does not differ too markedly, a second run through the wavelength list yields all lines giving coincidences with lines in the Multiplet Table. These lines are printed out in multiplet arrays, with various additional information on intensities, wavelength shifts, etc. If a line is used twice, this fact is indicated. In the same regions of the spectrum in which the machine program has been applied, Mrs. Littleton is pursuing the line identifications independently by the more familiar hand methods. It seems probably that the agreement between the two procedures will be satisfactory. To make sure of this last point, the entire Multiplet Table is

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presently being punched. When this punching, which is already well along, is completed, one will be able to make more systematic tests than have heretofore been possible. If the results of these more complete tests of the programs prove to be as successful as is presently hoped, it would appear that a significant amount of the heavy work of line identification in high dispersion spectra can be taken care of automatically. Consideration has been given to programs which might substantially reduce other portions of the work involved in the study of stellar spectra. The possibilities which such programs might open up for studies in a number of areas, for example, the range of properties of "normal" stars, are considerable.

Personnel:

Dr. Mabel Chen continued on three-fifths time and Mrs. Eleanor K. Kolchin on one-quarter time. Both salaries were shifted from an AEC contract to the NASA grant on November 1. Mrs. Norma C. Johnson continued on one-half time. Her salary was shifted from an ONR contract to NASA on November 1. Mrs. Cecily Littleton continued on one-fifth time on a NSF grant. Mr. Frank Ghigo, a Haverford undergraduate, continued to work on the project without salary as one part of his course load.

The Principal Investigator served as Provost of Haverford College and taught one course, "General Relativity and Cosmology", in the first semester. In August he was present at the Alberta Symposium on Quantum Chemistry at the University of Alberta in Edmonton. This conference was one of the most rewarding in the area of atomic and molecular calculations which the Principal Investigator has attended. In November, he attended the NASA Symposium on the Magnetic and other Peculiar and Metallic Line A Stars. An account of this meeting was prepared and appeared in the February issue of Sky and Telescope. In December, the Principal Investigator was present at the Miami Conference on the Observational Aspects of Cosmology. A report of this meeting has been written and will be published in the April issue of Sky and Telescope.